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THREE DIMENSIONAL FINITE ELEMENT STUDIES

PART ONE: SERVICE ROUTINES

by

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ABSTRACT:

In this report, service routines are developed for linear, quadratic and cubic finite elements for two and three dimensional regions. Also, an equation solver of very large capacity is developed for systems of linear equations where the matrix of coefficients is symmetrical, positive definite and tightly banded along the main diagonal.

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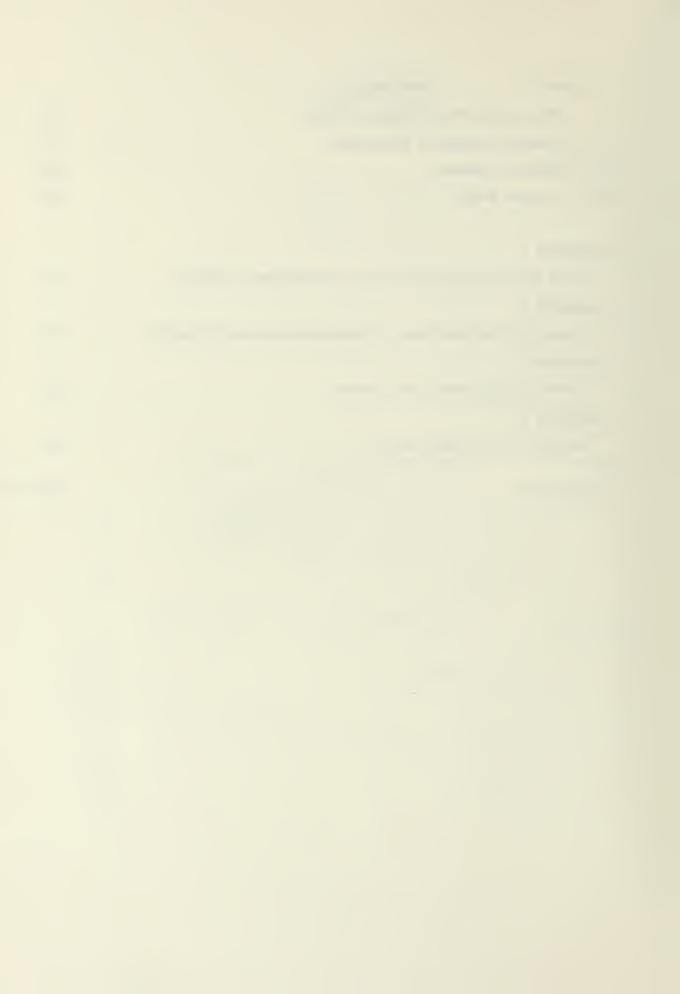


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INTRODUCTION

The stress-strain analysis of solid propellant rocket motors has been the object of numerous investigations in recent years. Various approximate methods of analysis have been proposed. The Finite Element method, without a doubt, showed the greatest promise of providing the information needed in the evaluation of real motors. In principle the method can provide analyses of any three dimensional bodies. Any number of material and geometrical discontinuities can be admitted. The method also allows for almost any type of static, dynamic and thermal loadings to be applied. In practice, however, this has proved to be a formidable computational task even for the largest digital computers in existence.

An elegant compromise was obtained with the development of axisymmetric ring elements (1)*. However this compromise eliminated the possibility of solving for real motors with star shaped grains. In those cases it has generally been assumed that a plane strain analysis using elements of triangular shape would provide enough information for design. The constant strain finite element triangle has been used ad nauseam in these studies, in spite of the fact that many other elements have been shown to provide much better results for the same computational effort (2). When the perforation changes shape, the combination of ring

^{*}Numbers in parenthesis refer to the reference list at the end.

elements and constant strain triangle cannot give reliable results.

Recently the introduction of isoparametric elements in the literature has given a new impetus to attempts at solving real three-dimensional motors (3), (4), (5). It is to such a task that we address ourselves. In this work we shall not attempt to account for real viscoelastic behavior, what we shall present is a linear elastic analysis method for three-dimensional objects. We will show that isoparametric elements can be economically generated in the computer, even for the monstrous (96×96) , 32 nodal point bricks. A massive system of linear equations with a large half-bandwidth normally results from the analysis of realistic problems. For these systems of equations we propose a new solver (6).

Chapter I. Isoparametric Elements

In this chapter we describe isoparametric elements and the numerical techniques used to construct them.

1.1 Advantages of isoparametric elements

The development of isoparametric elements marked an important breakthrough in the finite element method (4). Until then, a great variety of elements were developed to solve specific types of problems. The most successful elements satisfied all the requirements to insure convergence to an exact result by mesh refinement. However the solution of many problems required a combination of various elements which could not satisfy all the required conditions for successful convergence, when assembled to solve one problem. An example of such a situation is: an axisymmetric system where truncated conical ring elements are used to model a case around a rocket motor and ring elements of triangular cross section are used to model the grain (1). The usual conical element admits transverse displacements given by a cubic polynomial where as the grain ring elements will allow only linear displacement in the same direction. Obviously, adjacent ring and case elements cannot maintain continuity of displacements under strain.

Isoparametric element families on the other hand can be developed to yield compatible elements of any type: line, surface or volume.

Furthermore these elements admit curved boundaries, resulting in accurate modeling of complex shapes even with very few elements. The

results obtained in references (3), (4) and (5) show that good results are obtained with very coarse mesh.

1.2 Stiffness matrix of a finite element

The strain energy of an element having a stiffness matrix [K] can be written as:

$$U_{s} = \frac{1}{2} \langle \widetilde{u}_{i} \rangle [K] \{\widetilde{u}_{i}\}$$
 (1)

where the vector $\{\widetilde{u}_i^{}\}$ represents all the nodal coordinates of the element.

The same energy can also be written from fundamental principles as follows:

$$U_{s} = \frac{1}{2} \int_{V} \langle \sigma_{i} \rangle \{ \epsilon_{i} \} dv$$
 (2)

where $\{\sigma_i^{}\}$ is a vector of all the stress components and $\{\epsilon_i^{}\}$ a vector of corresponding strain components in the volume V. The constitutive laws can be written in matrix form as follows:

$$\{\sigma_{i}\} = [\varepsilon] \{\epsilon_{i}\} \tag{3}$$

where $[\mathcal{E}]$ is a symmetric matrix of material properties. The strain displacement relations are also written in matrix form as follows:

$$\{\epsilon_{i}\} = [\varphi] \begin{cases} u(x, y, z) \\ v(x, y, z) \\ w(x, y, z) \end{cases}$$

$$(4)$$

where matrix $[\phi]$ is in general a rectangular matrix of differential operators, and the vector $\langle u(x, y, z), v(x, y, z), w(x, y, z) \rangle^T$ represents

the three components of displacements in an appropriate global system of reference, (x, y, z). Finally the displacement functions are assumed to be of the following form:

$$\begin{cases} u(x, y, z) \\ v(x, y, z) \\ w(x, y, z) \end{cases} = [n] \{ u_i \}$$

$$(5)$$

where [n] is a rectangular matrix of carefully selected functions of (x, y, z). These functions must be selected to insure compatibility across common boundaries, to insure that rigid body motions will result in strainless states and finally to admit at least constant straining states.

After substitution of (5), (4) and (3) into (2) and using the definition:

$$[n^*] = [\varphi] [n] \tag{6}$$

we obtain the following result:

$$U_{s} = \frac{1}{2} \langle \widetilde{u}_{i} \rangle \left(\int_{V} [n^{*}]^{T} [e][n^{*}] dv \right) \{ \widetilde{u}_{i} \}$$
 (7)

The stiffness matrix is then:

$$[K] = \int_{V} [n^*]^{T} [\varepsilon][n^*] dv$$
 (8)

1.3 The isoparametric concept

In isoparametric elements, the displacements are obtained in terms of shape functions defined in a system of curvilinear coordinates particular to one element.

$$u(x, y, z) = N_{i}(\xi, \eta, \zeta)u_{i}$$

$$v(x, y, z) = N_{i}(\xi, \eta, \zeta)v_{i}$$

$$w(x, y, z) = N_{i}(\xi, \eta, \zeta)w_{i}$$
(9)

where $N_i(\xi,\eta,\zeta)$ are the shape functions and u_i , v_i , w_i are nodal values of the displacement components in the global system (x,y,z). The global system of reference is then related to the curvilinear coordinates by the same shape functions as follows:

$$x(\xi,\eta,\zeta) = N_{i}(\xi,\eta,\zeta) \times_{i}$$

$$y(\xi,\eta,\zeta) = N_{i}(\xi,\eta,\zeta) \times_{i}$$

$$z(\xi,\eta,\zeta) = N_{i}(\xi,\eta,\zeta) \times_{i}$$
(10)

where x_i , y_i and z_i are the nodal coordinates of the element in the global system (x, y, z). It is not our intention here to trace the history of such a concept. The readers are referred to references (3) and (4) for the details and justification of the concept. The remaining task is to construct the shape functions. We have taken these functions from reference (4). They will be found in section 1.6, 1.7 and 1.8.

1.4 The Jacobian Matrix

In equation (6), the derivatives of the shape functions in terms of the coordinates of the global system (x, y, z) are needed. These operations require the Jacobian of the transformation:

$$\left\{
\frac{\partial N_{i}}{\partial \xi} \right\} = \left\{
\frac{\partial x}{\partial \xi} \quad \frac{\partial y}{\partial \xi} \quad \frac{\partial z}{\partial \xi} \right\} \cdot \left\{
\frac{\partial N_{i}}{\partial x} \right\} = \left\{
\frac{\partial x}{\partial \eta} \quad \frac{\partial y}{\partial \eta} \quad \frac{\partial z}{\partial \eta} \right\} \cdot \left\{
\frac{\partial N_{i}}{\partial y} \right\} \cdot \left\{
\frac{\partial N_{i}}{\partial z} \right\} \cdot \left\{$$

where the square matrix is the Jacobian [J]. Using equation (10) the Jacobian matrix is easily evaluated as follows:

$$[J] = \begin{bmatrix} \frac{\partial N_1}{\partial \xi}, & \frac{\partial N_2}{\partial \xi}, & \dots \\ \frac{\partial N_1}{\partial \eta}, & \frac{\partial N_2}{\partial \eta}, & \dots \end{bmatrix} \begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \dots & \dots & \dots \end{bmatrix}$$

$$(12)$$

When the Jacobian is known the required derivatives are easily obtained. The element of volume is then transformed as follows:

$$dV = \det(J) d\xi d\eta d\zeta$$
 (13)

At this time everything is ideally suited for Gaussian numerical integration. This will be explained later.

1.5 Shape functions

As mentioned previously we take the displacement functions directly from reference (4). We write these shape functions for three dimensional

elements since they automatically contain the information for two and one dimensional elements. We also restrict our attention to tri-linear, tri-quadratic and tri-cubic polynomial expressions

1.6 Linear elements

The shape functions are:

$$N_{i} = \frac{1}{8} (1 + \xi_{o})(1 + \eta_{o})(1 + \zeta_{o}) i = 1, 2, ..., 8$$
 (14)

where $\xi_{0} = \xi \xi_{1}$ and ξ_{1} is ± 1 , similarly for η_{0} and ζ_{0} .

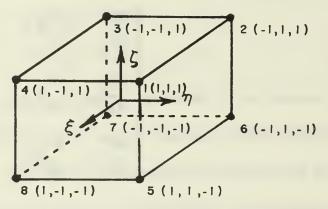


Figure 1. Linear element (8 nodal points)

1.7 Quadratic elements

See figure 2 for the identification of the nodal points.

Corner nodes: 1, 3, 5, 7, 13, 15, 17 and 19

$$N_{i} = \frac{1}{8} (1 + \xi_{0})(1 + \eta_{0})(1 + \zeta_{0})(\xi_{0} + \eta_{0} + \zeta_{0} - 2)$$
 (15)

where $\xi_{0} = \xi \xi_{1}$ and ξ_{1} is ± 1 , similarly for η_{0} and ζ_{0} .

Mid side nodes: 2, 6, 18 and 14

$$N_{i} = \frac{1}{4} (1 - \xi^{2}) (1 + \eta_{0}) (1 + \zeta_{0})$$
 (16)

Mid side nodes: 4, 8, 20 and 16

$$N_{i} = \frac{1}{4} (1 - \eta^{2}) (1 + \zeta_{0}) (1 + \xi_{0})$$
 (17)

Mid side nodes: 9, 10, 11 and 12

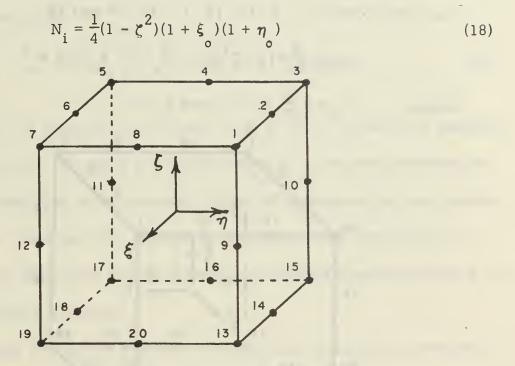


Figure 2. Quadratic element (20 nodal points)

1.8 Cubic elements

See figure 3 for the identification of the nodal points.

Corner nodes 1, 4, 7, 10, 21, 24, 27 and 30

$$N_{i} = \frac{1}{64} (1 + \xi_{0})(1 + \eta_{0})(1 + \zeta_{0})[9(\xi^{2} + \eta^{2} + \zeta^{2}) - 19] (19)$$

Mid side nodes: 2, 9, 29, 22, 3, 8, 28 and 23

$$N_{i} = \frac{9}{64} (1 - \xi^{2})(1 + 9\xi_{0})(1 + \eta_{0})(1 + \zeta_{0})$$
 (20)

where
$$\xi_i = \pm \frac{1}{3}$$
, $\eta_i = \pm 1$ and $\zeta_i = \pm 1$

Mid side nodes: 12, 32, 25, 5, 11, 31, 26 and 6

$$N_{i} = \frac{9}{64} (1 - \eta^{2})(1 + 9\eta_{0})(1 + \zeta_{0})(1 + \xi_{0})$$
 (21)

where

$$\eta_{i}=\pm\frac{1}{3}$$
 , $\xi_{i}=\pm$ 1 and $\zeta_{i}=\pm$ 1

Mid side nodes: 13, 14, 15, 16, 17, 18, 19 and 20

$$N_{i} = \frac{9}{64} (1 = \zeta^{2})(1 + 9\zeta_{0})(1 + \xi_{0})(1 + \eta_{0})$$
 (22)

where

$$\zeta_i = \pm \frac{1}{3}$$
, $\xi_i = \pm 1$ and $\eta_i = \pm 1$.

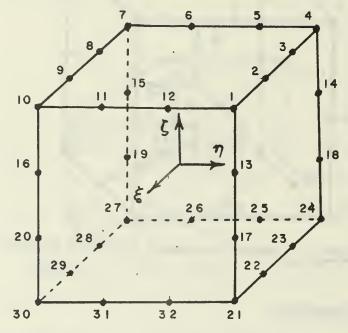


Figure 3. Cubic element (32 nodal points)

In all of these formulas if one coordinate , for example $\zeta=\zeta_0=1$, the formulas degenerate to the corresponding correct formulas for the two dimensional element in plane $(\xi,\,\eta)$. The same is true for line elements.

1.9 Numerical integration

When all the information contained in sections 1.4 to 1.8 is substituted into equation (8) we finally obtain an expression of the following form:

$$[K] = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} [k(\xi, \eta, \zeta)] d\xi d\eta d\zeta$$
 (23)

In this last expression the matrix $k(\xi, \eta, \zeta)$ is composed of elements in which the inverse of the Jacobian matrix is involved, furthermore, all the elements must be multiplied by the determinant of the Jacobian matrix. Obviously the process of reduction to the form shown in equation (23) is not trivial, however, a computational algorithm is not too difficult to obtain.

Once the form of equation (23) is obtained, Gaussian integration is straightforward. The number of Gauss points to be used in this integration is not easy to determine, especially if the element has irregular boundaries. For trirectangular elements, two, four and five Gauss ordinates in each direction of the local system of reference will give exact results for the linear, quadratic and cubic elements respectively. For elements having curved boundaries the same number of Gauss ordinates can only give approximate values to the stiffness matrix. We experimented with various numbers of Gauss points in those cases where the results were approximate, we observed that the dominant eigenvalues of the stiffness matrices were not sensitive

to the number of Gauss ordinates. We also observed that the trace of an approximate stiffness matrix was always smaller than the trace of the exact matrix. By increasing the number of Gauss points, the trace of the approximate matrix always approached the exact value from the low side. This error may actually be beneficial, since the trace of a stiffness matrix is known to be always greater than the trace of the actual stiffness of a real structure. For this reason we have adopted to use 2, 4 and 5 Gauss ordinates in the generation of the stiffness matrices. It will be necessary to show with actual problems whether or not this compromise is valid in general.

Chapter II. Computer Programs for the Generation of Stiffness Matrices

In this chapter we describe several computer programs used to evaluate the stiffness matrices of linear, quadratic and cubic elements for two and three dimensional bodies.

2.1 Stiffness matrices for two dimensional bodies

Appendix one contains the listing of a computer program that was used to evaluate the stiffness matrices of two-dimensional elements. Although the listing contains only one quadrature formula with five Gauss ordinates, an exhaustive series of tests was conducted with formulas using from two to ten Gauss ordinates. The five point formula was finally adopted for practical considerations; the formation times for one element were: 0.3, 1.0, 2.5 seconds for linear, quadratic and cubic elements respectively, and this was judged to be adequate for this phase of our research.

Following the strategy developed in section 1.9, two subroutines are needed to do all the work. The first subroutine named QUAD 5 performs the numerical integration, the second named FORMK assembles the stiffness matrix $k(\xi, \eta, \zeta)$ where (ξ, η, ζ) take their values at one of the Gauss points. Upon exit from the subroutines, the user will obtain the stiffness matrix of one of the elements in this family and also the transformation matrices between nodal strains (stresses) and nodal displacements. The calling statement is given in the appendix.

2.2 Stiffness matrices for three dimensional bodies

Appendix two contains three separate programs for the generation of the stiffnesses of linear, quadratic and cubic elements for three dimensional bodies. The three programs are similar in structure to the above program, they were coded separately for convenience during the testing phase of this study. The FORTRAN calling statements are all contained in the appendix. The number of Gauss point used was determined in section 1.9 for these elements.

Comments distributed throughout these programs should make the codes intelligible to an experienced user of finite element codes.

2.3 Numerical testing of stiffness matrices

The subroutines mentioned in the previous two articles were tested under the control of another program not listed here. Eigenvalues and eigenvectors were calculated for all these elements. Two dimensional elements always had three zero eigenvalues and three dimensional elements always had six zero eigenvalues. Static equilibrium checks were also applied to all elements and equilibrium was always satisfied.

2.4 Hybrid elements

A remarkable property of isoparametric elements is that once a high order element is obtained it can easily be degenerated to a lower order by simple matrix transformations. For example let us consider the eight nodal point two-dimensional element:

$$\{F\} = [K] \{\widetilde{u}_i\}$$
 (24)

where [K] is the stiffness matrix and $\{\widetilde{u}_i\}$ is the vector of nodal displacements;

$$\{\widetilde{\mathbf{u}}_{i}\} = \langle \mathbf{u}_{1}, \mathbf{v}_{1}, \mathbf{u}_{2}, \mathbf{v}_{2}, \mathbf{u}_{3}, \mathbf{v}_{3}, \mathbf{u}_{4}, \mathbf{u}_{4}, \mathbf{u}_{5}, \mathbf{v}_{5}, \mathbf{u}_{6}, \mathbf{v}_{6}, \mathbf{u}_{7}, \mathbf{v}_{7}, \mathbf{u}_{8}, \mathbf{v}_{8} \rangle^{T}$$
(25)

see figure 4.

To degenerate this element to the corresponding four nodal point element, it is only necessary to impose a simple constraint to the mid points of the element. If the mid-points are such that their nodal displacements are equal to the average of the displacements of their corresponding corner points the following transformation matrix is readily constructed:

$$\{\widetilde{\mathbf{u}}_{\mathbf{i}}\} = [T]\{\widetilde{\mathbf{u}}_{\mathbf{i}}^{*}\} \tag{26}$$

where

$$\{\widetilde{u}_{i}^{*}\} = \langle u_{1}, v_{1}, u_{3}, v_{3}, u_{5}, v_{5}, u_{7}, v_{7} \rangle^{T}$$
 (27)

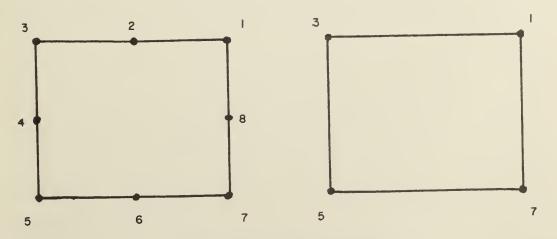


Figure 4. Hybrid elements

The matrix [T] in this case is simply:

	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	
	0.5	0.0	0.5	0.0	0.0	0.0	0.0	0.0	
	0.0	0.5	0.0	0.5	0.0	0.0	0.0	0.0	
	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	
	0.0	0.0	0.5	0.0	0.5	0.0	0.0	0.0	
[T] =	0.0	0.0	0.0	0.5	0.0	0.5	0.0	0.0	(28)
	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	. (20)
	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	
	0.0	0.0	0.0	0.0	0.5	0.0	0.5	0.0	
	0.0	0.0	0.0	0.0	0.0	0.5	0.0	0.5	
	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	
	0.5	0.0	0.0	0.0	0.0	0.0	0.5	0.0	
	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.5	

The stiffness matrix for the four nodal point element is simply:

$$[K^*] = [T]^T [K][T]$$
 (29)

If a five nodal point element is desired, for example, suppose we would like to keep nodal point 8 in the above example, then two columns would be added to the matrix [T]. Column 9 of [T] would have a one in row 15 and column 10 a one in row 16, all the other terms of rows 15 and 16 would be zeros. The congruent transformation (29) would give the stiffness of the hybrid element.

With such elements it is possible to combine different types of elements in the solution of one problem and still preserve all the conditions guaranteeing convergence to an exact result by mesh size reduction.

Chapter III. An Equation Solver of Very Large Capacity

In this chapter a very simple equation solver of very large capacity is developed. The method used does not require a very large incore memory; however, a fast random access device like a magnetic disk drive is required.

3.1 Introduction

The solution of very large systems of linear equations,

$$\{R\} = [K] \cdot \{r\} \tag{30}$$

where [K] is symmetric and positive definite, is an activity that must be entered by the stress analyst when using the finite element method. When the first automatic stress analysis programs were developed, the Gauss-Seidel iteration method, with various over relaxation schemes, was almost universally employed to solve the equations. It was soon realized that, because of the properties of [K], a direct Gaussian elimination algorithm would be much more economical of computer time. However, matrix [K], must be in core during elimination, and this puts a very stringent limitation on the total number of equations that can be solved.

For the purpose of comparing various methods, we will presume that we have at our disposition a machine with 32,000 words of core storage. Of the total memory, let us assume that approximately 25,000 words are available for the storage of [K]. For such a machine, then, approximately 160 equations, at most, can be solved by this

method.

Because the matrix [K] is usually sparse, a special ordering of the unknowns can produce a matrix [K] that is tightly banded about the main diagonal. Taking advantage of this character of [K], several programs were devised that required only (N.M) words for the storage of [K]. (See Figure 5 for the meaning of N and M). The short program listed in Appendix 3 is of that character. If M is very small, then the number of equations that can be solved can become fairly large. For example, using the same machine as above, if M = 50, then N = 500.

With the development of two and three dimensional elements, however, this improvement proved insufficient. These problems frequently lead to systems of several thousands of equations with a half band width in the hundreds. Equation solvers were then developed that did not require to have all the equations in core. Professor E. Wilson of the University of California at Berkeley (U. S.) several years ago developed a band solver that could be used with tape storage to solve large systems. The method used required (2M.M) words of in-core storage for [K] and the total number of equations that could be solved was only limited by the capacity of a tape. For the machine used above, the maximum value of M is approximately 110. Subsequently, as mentioned in Reference (8), several workers developed algorithms requiring only (M + 2)(M + 3)/2 words of core storage. For the machine

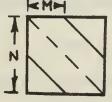
used above, the maximum value of M is approximately 220.

With large systems of equations, another difficulty becomes evident. Round off starts to play a very important role. An obvious remedy is to convert everything to double precision. However, this roughly doubles the core storage requirement. Round off can sometimes be eliminated by using the same programs to calculate corrections to the answer by an iterative technique. However, such corrections are not always valid when the matrix [K] is locally ill-conditioned. For this reason, many workers prefer to use double precision all the way. The block solver presented here uses double precision everywhere.

As mentioned in References (9) and (10), no method has been found that is faster and more accurate than Gaussian elimination for a system in which the matrix of coefficients is dense. For dense system banded along the main diagonal, it is reasonable to conjecture that the same conclusion will hold if the algorithm is modified to eliminate all operations involving the off diagonal zeros. Improvements can only be accomplished by taking advantage of the sparsity within the band, as shown in References (11) and (12). These improvements, however, are obtained at the cost of a more elaborate code to recognize the particular type of sparsity that can lead to important reductions of computations. The economies of storage, on the other hand, are not sufficient to allow for the solution of very large systems.

Frontal solvers, as described in References (13) and (8), also produce savings of storage and execution time, but again prohibit the solution of very large systems.

Our primary concern here was to design a solver that would permit the solution of very large systems even with a small computer. The block solver proposed in this paper does not pose any limits on the half band width nor on the total number of equations, as long as storage is available on a fast random access external device. The program contained in Appendix 4 requires 5800 bytes of storage for the object codes and a working space depending on the block size selected; for block sizes of (25, 50, 100) the storage requirements are (15600, 61200, 242400) bytes respectively. As mentioned above, a fast random access facility is required. In our computer center, we used IMB/2314 disk packs. On such a device, 55000 records, 400 bytes long, can be stored. This is enough for 2,750,000 double words. For example, 5000 equations with a half band width of 451 would fit with a complete load vector on one disk.



M is the half band width
N is the total number of
equations

Figure 5. Banded Character of K

^{*} A byte is a word segment of 8 bits of information.

3.2 Elimination by blocks

Consider the system of equations shown below:

The first equation is solved for r_1 to get:

$$r_1 = K_{11}^{-1} (R_1 - K_{12} r_2 - K_{13} r_3 - \dots - K_{1M} r_M)$$
 (32)

After substitution in equations 2 to M, we obtain the following results:

$$\overline{R}_2 = R_2 - K_{12}^T K_{11}^{-1} R_1$$
 (33)

$$\overline{R}_{M} = R_{M} - K_{1M}^{T} K_{11}^{-1} R_{1}$$
(34)

for the load vectors. All the coefficients in rows 2 to M from Column 2 to M are reduced by similar operations; a typical example for term K_{34} is:

$$\overline{K}_{34} = K_{34} - K_{13}^{T} K_{11}^{-1} K_{14}$$
 (35)

Then, Equation 2 is solved for r_2 and substituted in Equation 3 to M+1 and the entire process is repeated until we get only the last equation:

$$\overline{R}_{N} = \overline{K}_{NN} r_{N}$$
 (36)

This last equation can now be solved for $r_{\mbox{\scriptsize N}}$ and a simple process of back substitution in reverse order gives all the unknowns.

The elimination process described above preserves the symmetry of [K]. This process is valid, whether the elements of [K] are individual coefficients or square submatrices of coefficients. From now on, we presume that the $[K_{IJ}]$ are submatrices that we will call blocks. A careful examination of the elimination steps reveals that no more than three different blocks of coefficients are needed. With this in mind, the rest of the task is trivial. The simple solver contained in Appendix 3 was modified to do the elimination by blocks. Appendix 4 contains the listings of the four subroutines needed.

3.3 Listings

Subroutine SOLVE is self-explanatory and needs no elaboration, except as to the manner in which the equations must be stored. The blocks are stored sequentially by rows, as shown below. At the end of each row, a block of load vectors is present:

$$K_{11} K_{12} K_{13} K_{14} \dots K_{1m} R_{1}$$
 $K_{22} K_{23} K_{24} K_{25} \dots K_{2m} R_{2}$
 $K_{II} K_{I,I+1} \dots R_{I}$
 $K_{n-1,n-1} K_{n-1,n} K_{n-1}$
 $K_{nn} \dots K_{nn} K_{$

The symbols m and n are the number of blocks per row and column, respectively.

This method of storage leaves a few blocks of unused storage. However, the last row of blocks is needed for temporary storage during the elimination. Three service subroutines are needed in SOLVE. The multiplication and inversion operations are standard and need no words of explanation. The subroutine WRDISK/RDDISK, however, is hardware dependent and uses FORTRAN commands particular to IBM/360 installations (Reference 14). This feature, although undesirable, is not a very serious drawback because every installation using fast random access devices has specialized commands to use these facilities. For other installations, this subroutine would have to be rewritten to conform with the available hardware. The listings are self-explanatory.

3.4 Timing

The use of the program listed in Appendix 4 poses a serious practical problem. The solution of large systems of equations requires a large amount of computer time. The most important factors affecting the required time in the system proposed are: the number of calls to the WRDISK/RDDISK routine, and the size of the blocks (N_s) . In the program, the number of calls to WRDISK/RDDISK has been reduced as much as we could. In actual tests, the object codes were optimized, with respect to execution time, by the compilers that produced these object codes. We used the H compiler of release 18 of the IBM/360 operating system. A system of 500 equations with a half band width of 151 was solved with three different block sizes, (25, 50, 100). The execution times were (510, 402, 297) seconds, respectively. On the basis of this test, it seems that the block-size should be as large as the computer will allow, in order to reduce the execution time. For a block-size of 50, the following empirical formula gives an estimate of the required time:

 $T = 1.857 \text{ nm}^2 + 0.102 \text{ n}^2 \text{m} - 0.322 \text{ n}^2 + 4.682 \text{ nm} - 5.230 \text{ m}^2 \quad (38)$ The formula was obtained with the tests shown in Table 1. For the first test n = 4, m = 3, it was possible to obtain an in-core solution with the subroutine shown in Appendix 3. The execution time was 61.3 seconds for the in-core solution, as compared to 75.7 seconds for the block solver. This is indeed a very small penalty if we also compare the

storage requirements of the two solvers; 196K bytes for the in-core solver and 122K bytes for the block solver.

In a recent study, Reference (15), various equation solvers were compared. Using a sliding block technique similar to that mentioned in Reference (8), a system of 1080 equations with a half-band width of 357 was solved in 1365.1 seconds. The machine used was a CDC 6600 and the method used required 73728 words of core storage.

Test Number 5 in Table 1 shows that 1000 equations with a half-band width of 351 required 2989.8 seconds and used 15250 double words of core storage. Again, this is a comparison that seems very favorable to the block solver, if we keep in mind that the CDC6600 is a much faster machine than the IBM/360/67. Average execution times for division, multiplication and addition are: (2.9, 1.0, 0.4) microseconds for the CDC machine and (13.9, 10.6, 8.0) for the IBM machine.

3.5 Accuracy

The most critical operation, with respect to round-off, is the inversion of the diagonal blocks. If the block is singular, the program will print a diagnostic to this effect. However, this is not likely to happen very often. A much more serious difficulty comes from blocks that are nearly singular and this must also be detected. For this reason, the inversion routine will calculate an estimate of the round-off value of zero as the trace of the block multiplied by 10^{-12} and report that the block is nearly singular, if any diagonal term becomes smaller

TABLE 1 TIMING TESTS*

n (Number of blocks per column)	m (Number of blocks per row)	N (Number of equations)	M (Half-band width)	T (Time in seconds)
4	3	200	101	75.7
100	3	5000	101	2977.4
10	5	500	201	586.5
50	5	2500	201	3834.8
20	8	1000	351	2989.8

^{*}The blocksize used was 50 and the total storage requirement of the test program was 122K bytes or 15250 double words.

than this value during inversion. Besides these diagnostics, the program will also print a condition number for each diagonal block.

This condition number is obtained as the product of the maximum column sum of the block before and after inversion, following Wilkinson's perturbation theory. With this condition number, an estimate of the relative error in the answer can be obtained from:

$$E(\%) \le c \cdot \frac{\|P\|}{\|R\|} \cdot 100$$
 (39)

where c is the maximum value of all condition numbers of the system, $\|P\|$ is the sum of the absolute values of the estimated errors in the loads and $\|R\|$ is the sum of the absolute values of the loads.

3.6 Modifications

The program is presented in its simplest form; no facilities for iteration and multiple-load vectors are provided for. Users with particular needs should have no difficulty modifying the program listed, in order to take advantage of hardware available in their computing facilities.

3.7 <u>Conclusion</u>

The program presented here provides a very simple answer to a most difficult practical difficulty. When a problem is too big for a band or a frontal solver, the block solver will still give a solution, even with a very small computer, provided one is ready to pay a penalty in execution time.

Chapter IV. Conclusions

The publication of this report was delayed in order to verify the integrity of the service routines that it contains. This has now been completed and it can be reported that the routines perform as expected.

4.1 Stress-strain analysis codes

Several computer codes for mesh generation and consistent load vectors computation, as well as two basic stress strain programs for two and three dimensional problems, have been completed and tested (16), (17) and (18). From that work it may be concluded that these elements will shed significant new light on the stress analysis of rocket motors.

4.2 Reduced Gaussian Integration

In both reference (17) and (18), it is reported that the Gaussian integration mentioned in article 1.9 leads to improved results when only 2 and 3 Gauss ordinates are uses, respectively, in the generation of the 20 and 32 nodal point elements. This reduced integration also leads to significant economies in the total solution times.

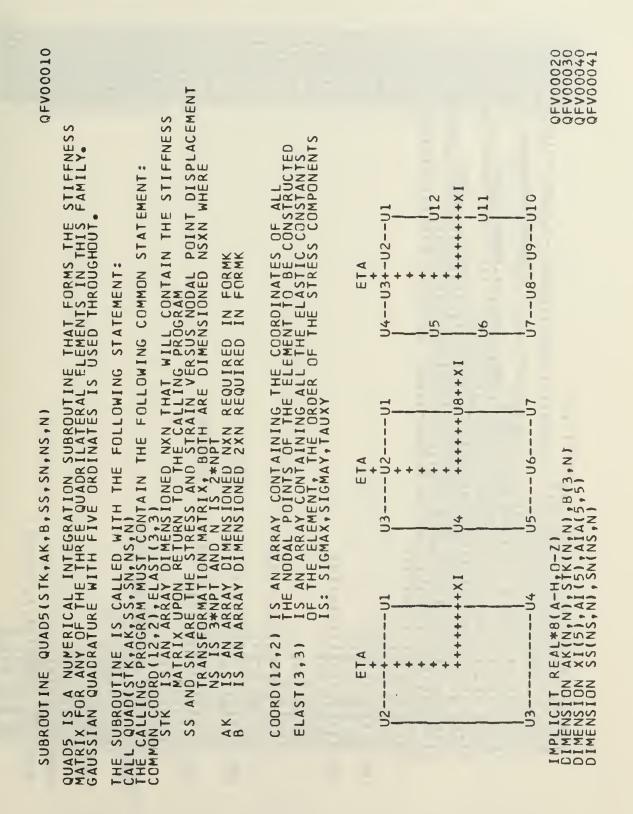
4.3 Surface stresses

In some problems it was observed that the stress and strain values obtained at the nodes were in error on the external surfaces of the objects analysed. Internal nodes, however, gave the best results. This matter deserves further investigations.

4.4 Future work

The program developed during the course of this investigation will be refined and released as soon as they are ready. In the meantime, potential users can refer to reference (17) for a first release of the three-dimensional programs.

Appendix I. Code for the generation of two-dimensional elements



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CCMMCN CCORD(12,2), ELASI(3,3)
DATA XI/0.9061798459386640,0.5384693101056831,0
156831,-0.9061798459386640,0.5384693101056831,0
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BOO AK(L,M)=AK(L,M)+ELAST(L,NN)*B(NN,M)

I = 3*(I-1)

I = 3*(I-1)

DO 900 J=1,3

I J=I I+J

DO 900 K=1,N

SS(IJ,K)=AK(J,K)

1C00 CONT INUE
RETURN
END

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DMY=DNE+Y

DMY=DNE-Y

DMY=DNE-Y

TMTMNX=3.000+2.0000*X-9.0000*X

TMTMNY=3.000-2.0000*Y-9.0000*X

TMTMNY=3.000-2.0000*X-9.0000*X

TMD=3.0000*Y-0NE

TXM0=3.0000*Y-0NE

TXM0=3.0000*Y-0NE

TXM0=3.0000*X-10NE

TXM0=3.0000*X-10NE

TXM0=3.0000*X-10NE

TXM0=3.0000*X-10NE

TXM0=3.0000*X-10NE

TXM0=3.0000*X-10NE

TMNMEY= 10.000-27.000*X-118

TMNMEX= 10.000-27.000*X-118
OPY=ONE+Y
OPX=ONE+X
OMX=ONE-X
WI (1.55) = OMY*TX PY /F OUR
WI (1.71) = OPY*TX PY /F OUR
WI (1.72) = OPY*TX PY /F OUR
WI (1.73) = OPY*TX PY /F OUR
WI (2.75) = OPY*TY PX /F OUR
WI (2.75) = OPX*TY PX /F OUR
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J=1,NPT
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K=1,2
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J=1,2
= ZERO
K=1,NPT
= AJ(I,J)+WI(I,K)*COORD(K,J)
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B1(I,J)=ZERC

B1(I,J)=B1(I,J)+B (K,I)*ELAST(K,J)

B0 500 K=1;3

B0 600 J=1,N

B0 600 J=1,N

B0 600 M=1;3

B0 700 J=1,N

B1(I,J)=AK(I,J)+B1(I,K)*B(K,J)

B1 700 J=1,N

B2 700 J=1,N

B3 700 J=1,N

B4 700 J=1,N

B4 700 J=1,N

B5 700 J=1,N

B6 700 J=1,N

B7 700 J=1,N

B7 700 J=1,N

B8 700 J=1,N

B9 7
DO 3CO I=1,NPT
IOD=2*I-1
IEV=2*I
B(1,100)=DNX(1,
B(2,1EV)=DNX(2,
B(3,1EV)=DNX(1,
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Appendix 2. Codes for the generation of three-dimensional elements

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COMMON CCCRD(8,3), ELAST(6,6)

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                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 IMPLICIT REAL*E(A-H,C-Z)

COMMON COORD(8,3)*ELAST(6,6)

CIMENSION XI(2)

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Appendix 3. Listing for an in-core band solver

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SUBROUTINE
                                                                                                                                                                                 ELEMENT
                                                                                                                    ELEMENT
                              THE COEFFICIENT MATRIX
THE RIGHT HAND MEMBER
A WORKING SPACE NEEDED IN THE SUI
THE TOTAL NUMBER OF EQUATIONS
THE HALF-BANDWIDTH OF THE SYSTEM
                                                                                                                                                                                  DIAGONAL
                                                                                                                    DIAGONAL
                                                                                                                                                                                                                               REMAINING EQUATIONS
                                                                                                                                                                                  ВУ
                                                                                                                                                   2. CHECK FOR LAST EQUATION
                                                                                                                    87
                                                                                                                                                                                EQUAT ION
SUBROUTINE SYMSOL(A,B,C,NN,MM)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION A(NN,MM),B(NN),C(MM)
                                                                                                                    SIDE
                                                                                                                                                                                                                                                                            DO 250 K=L, MM
J=J+1
A(I, J)=A(I, J)-C(L)*A(N,K)
B(I)=B(I)-C(L)*B(N)
CONTINUE
GO TO 100
                                                                                                                    1. DIVIDE RIGHT
                                                                                                    N TH EQUATION
                                                                                                                                                                                 三
                                                                                                                                                                                                                                              DO 260 L=2, MM
I=N+L-1
IF(NN-I) 260,240,240
                                                                                                                                                                 IF(N-NN) 150,300,150
                                                                                                                                                                                                DO 200 K=2, MM
C(K)=A(N,K)
A(N,K)=A(N,K)/A(N,1)
                                                                                                                                                                                                                                                                                                                                    SUBSTITUTION
                                                                                                                                                                                  Z
                                                                                                                                                                                                                               4. REDUCE
                                                                                                                                                                                 3. DIVIDE
                                                                                                                                   B(N)=B(N)/A(N,1)
                                SOSSOS
                                                                                                    REDUCE
                                                                                                                                                                                                                                                                                                                                   BACK
                               Z Z U M Z
                                                                              N=0
N=N+1
                                                                                                                                                                                                                                                                                                                                                   I-N=N
                                                                                                                                                                                                                                                                                                                                                   300
                                                                                      100
                                                                                                                                                                                                150
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C IF(N) 350,500,350

C 2. CALCULATE UNKNOWNS B(N)

C 350 D0 400 K=2, MM

L=N+K-1
IF(NN-L) 400,370,370

370 B(N)=B(N)-A(N,K)*B(L)

400 CONTINUE
60 T0 300

500 RETURN
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Appendix 4. Listing for the Block Solver

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ZZZZZZZZ
SLV00110
SLV00120
SLV00130
                                                                                                                                                      SLV00150
SLV00150
SLV00150
SLV001170
SLV00170
SLV000220
SLV000244
SLV000244
SLV000240
SLV000340
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                           DECEMBER
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                           360/67
                                                                                                                                                                                                                                        NEARLY
                                                                                                                                                                                                                                                                          BLOCKS
                           GILLES
AN IBM
                                                                                                                                                                                             NTK=NTRK(N,1)

NTR=N*(MM+1)

CALL RDDISK(NTK, AK2, NC OUNT)

CALL SYMINV(AK2, NS, RB1, RB2, IFLG)

IF(IFLG.EQ.1) GO TO 600

IF(IFLG.EQ.2) WRITE(6, 2000) N

IF(IFLG.EQ.2) WRITE(6, 2000) N

CALL RDDISK(NTR, RB1, NS)

CALL MULT(AK2, RB1, RB2, NS, NS, 1)

CALL WRDISK(NTR, RB2, NS, NS, 1)
                                                                                                                                                                                                                                                                                                     :
Z
:
                                                                                                                                                                                                                                                                          9
                                                                                                                                                                                                                                                                                                     ROM
SOLVE(NN, MM, NS)
EAL*8(A-H, D-Z)
***********
                                                                                                                                                                                                                                                                                                                   F(N.GT.(NN-MM+1)) KMM=KMM-1
                          BY:
                                                                                                                                                                                                                                                                          ROM
                           CODED BY
                                                                                                                                                                                                                                                                                                     BLOCKS IN
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BLOCKS
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                                                                                                                                                                                                         DD 260 L=2,KMM

I=N+L-1
IF(I.GT.NN) GD TD 260

NTK=NTRK(NN,L)
CALL RDDISK (NTK,AK1,NCOUNT)
CALL RDDISK(NTK,AK1,NCOUNT)
CALL WRDISK(NTK,AK1,NCOUNT)
CALL WRDISK(NTK,AK1,NCOUNT)
CALL MRDISK(NTK,AK1,NCOUNT)
CALL MULT(AK2,RB2,RB3,NS,NS,1)
NTR=I*(MM+1)
CALL MULT(AK2,RB2,RB3,NS,NS,1)
CALL WRDISK(NTR,RB1,NS)
CALL WRDISK(NTR,RB1,NS)
CALL WRDISK(NTR,RB1,NS)
CCONTINUE
CALL WRDISK(NTR,RB1,NS)
CCONTINUE
CALL WRDISK(NTR,RB1,NS)
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SK(NTK, AK1, NCOUNT)
(AK2, AK1, AK3, NS, NS)
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                                                                                                                                                                                     REDUCE
DD 200 K=2, KMM
NTK=NTRK(N,K)
CALL RDDISK(NT)
CALL WRDISK(NT)
DD 150 1=1, NS
TI=(I-1)*NS
DD 150 J=1, NS
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          CHECK
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IREI+(1-1)
AK3(IL)=AK
NTK=NTRK(N
CALL WRDIS
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                                OF UNKNOWNS
                                                  NT1=N*(MM+1)
CALL RDDISK(NT1,RB3,NS)
DO 400 K=2,KMM
L=N+K-1
IF(L.6T.NN) GO TO 400
NTK=NTRK(N,K)
CALL RDDISK(NTK,AK1,NCOUNT)
NTREL*(MM+1)
CALL RDDISK(NTR,RB1,NS)
CALL MULT(AK1,RB1,NS)
CALL MULT(AK1,RB1,NS)
CALL MULT(AK1,RB1,NS)
CALL MULT(RM+1)
CALL MRDISK(NT1,RB3,NS)
KWM=KMM+1
IF(KMM.GT.MV) KMM=MM
GO TO 300
NRITE(6,1000) N
WRITE(6,1000) N
STOP
END
                                                                                                                                                                                                                                                                 SI
                                CALCULATE BLOCKS
          (N.EQ.0) GO TO 500
                                 2.-
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500

310

MLT00020 MLT00020 MLT000030 MLT000040 MLT000080 MLT000130 MLT001130 MLT001130

SUBROUTINE MULT(A,B,C,NRA,NCA,NCB)
IMPLICIT REAL*8(A-H,0-Z)
DIMENSION A(1),8(1),C(1)
ZRO=0.000
DO 100 I=1,NRA
DO 100 J=1,NRA
C(IC)=ZRO
IOO ZRO

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    C, IFLG
      MATRIX INVERSION
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                                                   ZRO)
D).L
=1.N
J)/O
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                                              J=1 + N
                                              DD 100 J=1
K=NR+J
B(J)=A(K)
D=B(I)
IF(D•EQ•ZR
IF(DABS(D)
DO 110 J=1
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                                                                                                                                     WRITE
                                                                                                                                                                                                                                                                                                                                                                                                                                            ON AN IBM/2314 D
280,460) FOR NS
THIS IS A DIRECT ACCESS SUBROUTINE TO READ OR NS IS THE SAME PARAMETER AS USED IN SOLVE NRECORD IS THE LENGTH OF ONE RECORD, IT MUST BINAMAX IS THE MAXIMUM NUMBER OF RECORDS IT MUST (THE PARAMETERS NN AND MM ARE THE SAME AS
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AST+NRL-1)/NR
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NRMAX //NC, WHERE NC IS (120 (100,50,25) RESPECTIVELY.
                                                                                                                                                                                                                                                                                                                                                                                                       Z
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                , J=1, NRL)
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                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         T0 =
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AST = I
LAST=0
                                                                                                                                                                                                                                                                                                                                                                                                       OF.
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      NRCD ) GO
O) NTRACK
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                ,1000) (A(J)
NRL - 1
                                                                                                                                                                                                                                                                                                                                                                                                       NUMBER
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1000) (A
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                                                                                                                                                                                                                                                 THE (
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    DEFINE FILE 7(20)
NRCM=2000
FORMAT (50AR)
NRCM=NRCM-1
NRCD=NRCM/NRL
IF(NTRACK 6T.0
IF(NTRACK 6T.0
N=N*NRL+1
IF(NTRACK-1
N=N*NRL+1
IF(NCT-6T.00)
IF(LAST-6T.NRL)
IF(NRCM-1000)
IF
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                                                                                                                                                                                                                                                 CHANGE T
ZZZZ
ZZZZ
NRMAX
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BE
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                                                                                                                                                                                                              ,NRCD,NTRACK
ALL OF ',A6,',
= ',I5)
IF ( JE .GE .NCT) GO TO 100
WRITE (7'I;1000) (A(J),J=JI,JE)
JI = JI + NRL
GO TO 75

O WRITE (7'I;1000) (A(J),J=JI,NCT)
IF(I .GT .LAST) LAST=I
IF(LAST.GT .NRCMM)LAST=O
RETURN
RETURN
RETURN
RETURN
IF(NTRACK .GT.NRCD) GO TO 910
IF(NCT.GT.NRCD) GO TO 910
IF(NCT.GT.NRC) (B(J),J=I,NCT)
READ (7'N,1000) (B(J),J=I,NRL)
RETURN
RETURN
O READ (7'N,1000) (B(J),J=I,NRL)
                                                                                                                                                                           (7'I,1000) (B(J),J=JI,NCT)
                                                                                                                                              GO TO 200
(B(J), J=JI, JE
                                                                                                                                                                                                30 TO 920
                                                                                                                                                                           READ
RETURN
K=1
                                                                                                                                                                           200
                                                                                                                                                                                         006
                                                                                                                                                                                                       910
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In this report, service routines are developed for linear, quadratic and cubic finite elements for two and three dimensional regions. Also, an equation solver of very large capacity is developed for systems of linear equations where the matrix of coefficients is symmetrical, positive definite and tightly banded along the main diagonal.

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KEY WORDS	ROLE	WT	ROLE	WT	ROLE	WT
Isoparametric						
Finite Elements						
Computer Code						
Linear Equation Solver						
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